Where do all the Supercurvature Modes Go?

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In the hyperbolic slicing of de Sitter space appropriate for open universe models, a curvature scale is present and supercurvature fluctuations are possible. In some cases, the expansion of a scalar field in the Bunch-Davies vacuum includes supercurvature modes, as shown by Sasaki, Tanaka and Yamamoto. We express the normalizable vacuum supercurvature modes for a massless scalar field in terms of the basis modes for the spatially-flat slicing of de Sitter space.

I. INTRODUCTION

Scalar fields in de Sitter spacetime have long provided a testing ground for issues of quantum field theory in curved spacetime [1,2]. Further motivation for their study stems from the central role they play in inflationary cosmology [3]. Several different coordinate systems can be used to cover de Sitter space, and subtleties in the quantization of fields can arise in some of the less familiar coordinate systems. These subtleties have been highlighted by recent models of open inflation [4,5], in which two periods of inflation are separated by nucleation of a bubble. The bubble interior includes an open universe ($\Omega_0 < 1$), where we could be living today, described by hyperbolic, spatially-curved coordinates [6].

A key difference between these hyperbolic coordinates and the more familiar spatially-flat slicing of de Sitter space is the presence of a curvature scale. This in turn leads to the possibility of supercurvature [7] fluctuations, fluctuations with wavelength longer than the curvature scale. Unlike the continuum of modes familiar from the spatially-flat slicing of de Sitter space, a normalizable supercurvature mode may exist for an isolated, discrete eigenvalue of the spatial Laplacian, or not at all. Although such modes have no analogue in the spatially-flat slicing of de Sitter space, it has been shown [8] (see also [9]) that the supercurvature modes must be included in the vacuum spectra of low-mass scalar fields in order to produce a complete set of states, and hence the proper Wightman function.

For massless, minimally-coupled scalar fields in de Sitter space, there is in addition a well-known infrared divergence in the (coordinate-independent) Wightman function. The infrared divergence is related to a dynamical zero mode in the spectrum of a massless field [10,11]. Kirsten and Garriga [11] covariantly quantized this zero mode in a spatially-closed slicing of de Sitter space. Extending their result from these closed coordinates to the coordinate system

1

appropriate to open inflation has not yet been done. Here we identify the zero mode as one of the supercurvature modes when quantizing the minimally-coupled massless field in the open hyperbolic coordinates.

It has already been noted that supercurvature modes can make significant contributions to the fluctuations in the cosmic microwave background (CMB) radiation, and several of their effects have been calculated for models of open inflation [12–15]. (The massless field zero-mode subtleties, except for a variant studied in [15], do not arise for these specific CMB calculations, which are sensitive to higher multipoles.) In addition to contributing to observable density fluctuations, such long wavelength, supercurvature modes might play a role [16] at the end of inflation, when recent advances [17] in the theory of reheating are taken into consideration.

In summary, increased understanding of these supercurvature modes is motivated both by general questions of quantizing fields in curved backgrounds, and by recent inflationary model-building. We will focus here on the example of supercurvature modes for a massless, minimally-coupled scalar field, expressing them as a sum over the basis modes for a spatially-flat slicing of de Sitter space. This overlap gives a measure of "where all the supercurvature modes go" in the familiar flat-space spectrum of such fields. The massless case is chosen for tractability, and questions about the zero mode are postponed for future work [18].

Throughout this paper, we consider only an unperturbed de Sitter metric; a more complete treatment would include study of the backreaction of such fields on the background metric. Because the supercurvature modes stretch beyond the horizon, any such study of the coupled metric fluctuations would need to pay special attention to the gauge subtleties which always accompany superhorizon fluctuations [19], and such issues are not pursued here.

In section II, the two covers of de Sitter space (including the flat and hyperbolic slicings) are given, and the field quantization pertinent to open inflation in both systems is reviewed. As these supercurvature modes have no analogue in the usual flat slicing of de Sitter space, this section gathers some previous work on supercurvature modes and provides notation and context for the rest of the paper. Section III specializes to the massless case. The explicit calculation of the overlap for some of these supercurvature modes and the more familiar flat space modes is given, and indicates a general form for the overlap between all the massless supercurvature and spatially flat modes. We verify this general form by integrating over the spatially flat modes, weighted by the overlap, to obtain the original supercurvature modes. Concluding remarks follow in Section IV. Three Appendices include the supercurvature mode normalization at fixed time in the flat coordinates, and details of the overlap calculation along different hypersurfaces within de Sitter space.

II. DE SITTER SPACETIME AND SCALAR FIELD QUANTIZATION

We begin by considering de Sitter spacetime as embedded within a 5-dimensional Minkowski spacetime, with the five coordinates subject to the constraint [1]:

$$- \left(z^0\right)^2 + \sum_{i=1}^{4} \left(z^i\right)^2 = 1. \tag{1}$$

The radius of the embedded spacetime, H^{-1}, is scaled to unity.

A spatially flat slicing (see, *e.g.* [1]) which partially covers the resulting 4-dimensional de Sitter spacetime is

$$z^0 = \sinh t_f + \frac{1}{2} e^{t_f} r_f^2 = -\frac{1}{2\eta} \left(1 + r_f^2\right) + \frac{1}{2}\eta,$$

$$z^4 = \cosh t_f - \frac{1}{2} e^{t_f} r_f^2 = -\frac{1}{2\eta} \left(1 - r_f^2\right) - \frac{1}{2}\eta,$$

$$\vec{z} = e^{t_f} r_f \vec{\Omega} = -\frac{r_f}{\eta}\vec{\Omega}, \tag{2}$$

where $\vec{\Omega} \equiv (\sin\theta\cos\varphi, \ \sin\theta\sin\varphi, \ \cos\theta)$, and conformal time $d\eta = a^{-1}dt_f$, or $\eta = -a^{-1}(t_f) = -e^{-t_f}$. Here $r_f \geq 0$, $-\infty < \eta \leq 0$. (See Figure 1.)
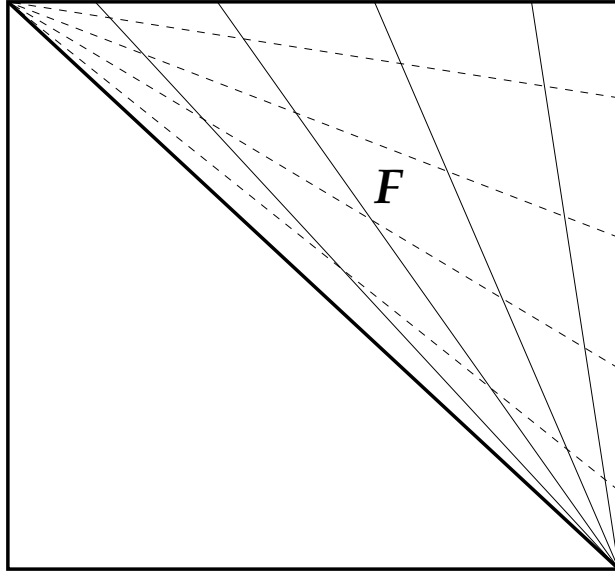

FIG. 1. De Sitter spacetime as covered by the coordinates in equation (2). Solid lines are lines of constant r, and dashed lines are lines of constant η.

The metric on this portion of the spacetime is

$$ds_f^2 = \eta^{-2} \left[-d\eta^2 + dr_f^2 + r_f^2 d\Omega^2\right], \tag{3}$$

where $d\Omega^2 \equiv d\theta^2 + \sin^2\theta d\varphi^2$. The coordinates x_f and metric ds_f^2 are useful in ordinary models of inflation, in which the spatial curvature quickly becomes completely negligible. These coordinates x_f cover only that half of the total spacetime with $z^0 + z^4 \geq 0$. Replacing $z^4 \to -z^4$ in the above produces a second flat coordinate system.

In contrast, for models of open inflation, open hyperbolic coordinates are appropriate inside the open universe. This coordinate patch is part of the full de Sitter spacetime (discussed in detail by [8,20]) as shown in Figure 2.
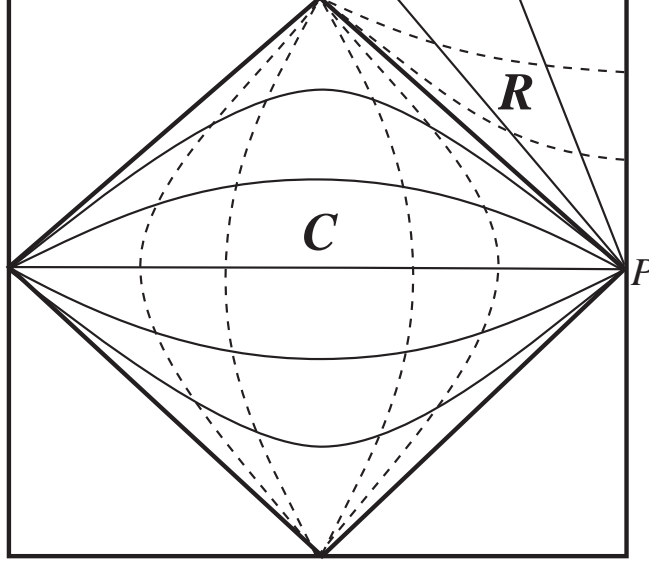
FIG. 2. De Sitter spacetime as covered by the coordinates in equation (4). Solid lines are lines of constant r, and dashed lines are lines of constant t. If a (thin-walled) bubble nucleated with center at point P, then region R, the forward light cone of point P, would contain in the interior of the nucleated bubble. In models of open inflation, region R would contain our observable universe at some time t inside the light cone corresponding to $t = 0$.

The two most important of these regions for our purposes here are region C, a large, compact subspace, and region R, an open hyperboloid bordering region C. These are related to the embedding coordinates by

$$z^0 = \cos t_c \sinh r_c = \sinh t_r \cosh r_r,$$

$$z^4 = \sin t_c = \cosh t_r,$$

$$\vec{z} = \cos t_c \cosh r_c \vec{\Omega} = \sinh t_r \sinh r_r \vec{\Omega}. \tag{4}$$

These coordinates lie in the ranges

$$-\frac{\pi}{2} \leq t_c \leq \frac{\pi}{2} \ , \ \ -\infty < r_c < \infty \ \text{and} \ \ 0 \leq t_r \ , \ \ 0 \leq r_r, \tag{5}$$

and are related by the analytic continuation $t_r = it_c - \frac{i\pi}{2}$ and $r_r = r_c + \frac{i\pi}{2}$. The corresponding metrics are

$$ds_c^2 = dt_c^2 + \cos^2 t_c \left[-dr_c^2 + \cosh^2 r_c d\Omega^2 \right],$$

$$ds_r^2 = -dt_r^2 + \sinh^2 t_r \left[dr_r^2 + \sinh^2 r_r d\Omega^2 \right]. \tag{6}$$

Note that r_c plays the role of 'time' within region C.

The forward light cone of the point P in Figure 2 is the center of the nucleated bubble in models of open inflation, so that region R contains the spatially-open universe we may be in today. Region C is of interest because surfaces of

fixed time, $r_c =$ constant, correspond to Cauchy surfaces for de Sitter space.[1] Quantizing on a Cauchy surface in C thus specifies all of the "initial data" for the system, including the initial conditions for the spatially-open universe inside region R.

The equation of motion for a scalar field of mass M in this space is

$$\left(\Box - M^2\right)\phi(x) = \left((\sqrt{-g})^{-1}\partial_\mu\left[(\sqrt{-g})g^{\mu\nu}\partial_\nu\right] - M^2\right)\phi(x) = 0, \tag{7}$$

and separation of variables gives a family of solutions $\phi_{k\ell m}(x)$. To quantize, ϕ and its canonically conjugate momentum Π are promoted to Heisenberg operators, and expanded as

$$\hat{\phi}(x) = \sum_{k\ell m}\left[\phi_{k\ell m}(x)\hat{a}_{k\ell m} + \overline{\phi}_{k\ell m}(x)\hat{a}_{k\ell m}^\dagger\right] \tag{8}$$

and similarly for $\hat{\Pi}$. The creation and annihilation operators satisfy $[\hat{a}_{k\ell m}, \hat{a}_{k'\ell'm'}^\dagger] = \delta(k-k')\delta_{\ell'\ell}\delta_{m'm}$ with the other commutators vanishing. Here an overline denotes complex conjugation, $\sum_{k\ell m}$ is a placeholder for the appropriate measure, and the choice of vacuum state satisfying $\hat{a}_{k\ell m}|0\rangle = 0$ for all (k, ℓ, m) provides a division into positive and negative frequency modes. The fixed-time canonical commutation relations, $[\hat{\phi}(x), \hat{\Pi}(x')] = i\delta^3(\vec{x} - \vec{x}')$ then imply that

$$(\phi_{k\ell m}, \phi_{k'\ell'm'}) = \delta(k-k')\delta_{\ell'\ell}\delta_{m'm} \ , \ \ (\phi_{k\ell m}, \overline{\phi}_{k'\ell'm'}) = 0 \ ,$$
$$(\overline{\phi}_{k\ell m}, \overline{\phi}_{k'\ell'm'}) = -\delta(k-k')\delta_{\ell'\ell}\delta_{m'm}, \tag{9}$$

where the Klein-Gordon inner product is defined by

$$(\phi_{k\ell m}, \phi_{k'\ell'm'}) \equiv -\int_\Sigma \left(\phi_{k\ell m} \overset{\leftrightarrow}{\partial_\mu} \overline{\phi}_{k'\ell'm'}\right)\sqrt{-g_\Sigma}\, n^\mu\, d\Sigma\,. \tag{10}$$

Here Σ is a (spacelike) Cauchy surface and n^μ is a future-directed unit vector normal to this surface. (The extra factor of i which multiplies the righthand side of equation (10) in [1] is absent here because of our different sign convention for the metric.) This inner product is independent of Cauchy surface, and more generally is independent of the choice of Σ, as long as the fields fall off sufficiently quickly on the time-like boundaries.

The physically-motivated choice of initial vacuum state in models of inflation is the Bunch-Davies vacuum [22], which respects the symmetries of de Sitter space and reduces to the Minkowski space vacuum at early times and over short distances. For the flat slicing, the Bunch-Davies positive-frequency modes are

$$\phi_{k\ell m}(x_f) = \frac{k}{\sqrt{2}}\exp\left[i\frac{\pi}{2}\left(\nu+\frac{1}{2}\right)\right]\frac{(-\eta)^{1/2}}{a(\eta)}H_\nu^{(1)}(-k\eta)j_\ell(kr_f)Y_{\ell m}(\Omega), \tag{11}$$

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[1] A Cauchy surface is any hypersurface such that every future-directed time-like vector intercepts it exactly once. (See, *e.g.*, [21].)

where $\nu \equiv \sqrt{\frac{9}{4} - M^2}$, $H_\nu^{(1)}(z)$ is a Hankel function of the first kind, $j_\ell(z)$ is a spherical Bessel function, and $Y_{\ell m}(\Omega)$ is the usual spherical harmonic. The measure in equation (8) for the expansion in flat modes $\phi_{k\ell m}$ is $\sum_{k\ell m} = \int_0^\infty dk \sum_{\ell=0}^\infty \sum_{m=-\ell}^\ell$.

For the hyperbolic slicing with the metric ds_c^2 of equation (6), the positive-frequency solutions to the equations of motion are [4,8,23]

$$u_{p\ell m}(x) = \frac{\chi_p(t_c)}{a(t_c)} f_{pl}(r_c) Y_{\ell m}(\Omega), \tag{12}$$

where

$$\chi_p(t_c) = \alpha_p(\nu') P_{\nu'}^{-ip}(\sin t_c) + \beta_p(\nu') P_{\nu'}^{ip}(\sin t_c) ,$$
$$f_{p\ell}(r_c) = \frac{P_{ip-1/2}^{-\ell-1/2}(i \sinh r_c)}{\sqrt{i \cosh r_c}}, \tag{13}$$

and

$$\nu' \equiv \nu - \frac{1}{2} = \sqrt{\frac{9}{4} - M^2} - \frac{1}{2} . \tag{14}$$

Here $P_\nu^\mu(z)$ is an associated Legendre function of the first kind, while the specific forms of α_p, β_p will not be needed. Within region C, the $f_{p\ell}(r_c)$ play the role of positive-frequency solutions, and the $\chi_p(t_c)$ are spatial eigenfunctions; when continued into region R, these roles are reversed.

A Friedmann-Robertson-Walker metric with spatial curvature K and cosmic scale factor $a(t)$ has a physical curvature length scale $a(t)/|K|$. For a flat universe the comoving curvature length scale thus runs off to infinity, whereas in a spatially closed or open metric, the comoving curvature length scale is $+1$. Eigenvalues of the (region R) spatial Laplacian in this background are $-(k/a)^2$, where (k/a) is the inverse of a physical length: $k/a = 1/x_{\text{phys}}$, with $0 \le k^2 < \infty$. Defining $p^2 \equiv k^2 - 1$, $p^2 > 0$ for subcurvature modes, and $-1 < p^2 \le 0$ for supercurvature modes. The continuum of subcurvature modes $0 \le p \le \infty$ is sufficient to describe a Gaussian random field in region R, see [7] for detailed discussion. In addition, for $p^2 < 0$, inner products of the form (10) on fixed-time (non-Cauchy) surfaces within region R diverge, and so all supercurvature modes naively appear to be unnormalizable. Studying quantization and completeness more appropriately on a fixed time r_c Cauchy surface in region C, it was found in [8] that for $M^2 < 2H^2$ (restoring the Hubble radius, H^{-1}), supercurvature modes are normalizable in vacuum for a discrete value of p. In addition, it was shown there that this value of p must be included to obtain the correct Wightman function for the Bunch-Davies vacuum. (See also [9].)

This discrete normalizable supercurvature mode can be understood as follows [8,23]. Its presence is suggested by an analogy between these supercurvature modes and bound states in a potential. The only dependence on M in the wavefunctions is in the 'spatial' (in region C) eigenfunctions $\chi_p(t_c)$. Defining $\sin t_c \equiv \tanh u$, the equation of motion for χ_p becomes

6

$$\left[-\frac{d^2}{du^2} + U(u) \right] \chi_p = p^2 \chi_p \, ,$$

$$U(u) \equiv \frac{M^2 - 2}{\cosh^2 u}. \tag{15}$$

This is a one-dimensional Schrödinger-like equation with the potential $U(u)$ and energy p^2. As noted in [13,14,23], the potential $U(u)$ vanishes as $u \to \pm\infty$, revealing that in this limit there exists a continuous spectrum of modes with $p^2 \geq 0$. But over finite intervals of u, if the mass of the field satisfies $M^2 < 2$, the potential $U(u)$ has a valley and the modes χ_p behave as discrete bound states with $p^2 < 0$. As DeWitt has shown, such discrete states in a field's spectrum are generic for fields quantized on compact subspaces. [24]

The inner product on this space is proportional to

$$\int_{-\infty}^{\infty} du \, \chi_p(\tanh u) \overline{\chi}_{p'}(\tanh u) \, , \tag{16}$$

so for normalizability, $\chi_p(\tanh u)$ must be bounded as $u \to \pm\infty$. (A similar argument is found in the appendix of [8].) A supercurvature mode has $p^2 < 0$ and $p^2 + 1 \geq 0$, so define $p = i\Lambda$, with $0 \leq \Lambda \leq 1$, and Λ real. The asymptotics of χ_p near $\tanh u \to \pm 1$ yields (cf. [23]):

$$\Gamma(1 \mp ip) P_{\nu'}^{\pm ip}(\tanh u) \sim e^{\pm ipu} \, , \quad u \to \infty. \tag{17}$$

This is finite only for $P_{\nu'}^{+ip}$ since $ip = -\Lambda < 0$, thus $\beta_p = 0$ for the supercurvature modes. The limit of $P_{\nu'}^{ip}(\tanh u)$ as $u \to -\infty$ is [23][2]

$$\Gamma(1 + \Lambda) P_{\nu'}^{-\Lambda}(\tanh u) \sim \frac{\Gamma(1 + \Lambda)\Gamma(\Lambda)}{\Gamma(1 + \nu' + \Lambda)\Gamma(\Lambda - \nu')} e^{\Lambda|u|} + \frac{\Gamma(1 + \Lambda)\Gamma(-\Lambda)}{\Gamma(-\nu')\Gamma(1 + \nu')} e^{-\Lambda|u|} \, , \quad u \to -\infty. \tag{18}$$

As $0 < \Lambda \leq 1$ is non-negative and $0 \leq \text{Re } \nu' \leq 1$, the coefficient of $e^{\Lambda|u|}$ vanishes only if $\Lambda = \nu'$, producing an isolated value of p which is normalizable. (Note that for subcurvature modes, with p real and non-negative, the solution $\chi_p(t_c)$ simply oscillates at both endpoints and so remains finite.)

The Klein Gordon normalized supercurvature modes are then

$$u_{\Lambda \ell m}(x_c) = N_{\Lambda \ell m}(-i \cos t_c)^{\nu' - 1} \frac{P_{-\Lambda - 1/2}^{-\ell - 1/2}(i \sinh r_c)}{\sqrt{i \cosh r_c}} Y_{\ell m}(\Omega),$$

$$N_{\Lambda \ell m} \equiv \left[\frac{\Gamma(\nu' + 1/2)\Gamma(-\nu' + \ell + 1)\Gamma(\nu' + \ell + 1)}{2\sqrt{\pi}\Gamma(\nu')} \right]^{1/2} . \tag{19}$$

The scalar field in region C is expanded as [8]

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[2]Note that in the derivation of this result in [23], their equation (2.9) is incorrect, including only the factor $w^{-\mu}$ instead of $[(1 - w)/w]^\mu$, though their next equation is correct.

$$\hat{\phi}(x_c) = \int_0^\infty dp \sum_{\ell,m} [u_{p\ell m}(x_c)\hat{a}_{p\ell m} + \text{H.c.}] + \sum_{\ell,m} [u_{\Lambda\ell m}(x_c)\hat{a}_{\Lambda\ell m} + \text{H.c.}]$$

$$\equiv \hat{\phi}_{(p)}(x_c) + \hat{\phi}_{(\Lambda)}(x_c), \tag{20}$$

where "H.c" denotes the Hermitian conjugate, and $\sum_{\ell,m} \equiv \sum_{\ell=0}^\infty \sum_{m=-\ell}^\ell$. Once quantized, these modes may be continued into region R. In the presence of a bubble wall [14], rather than in the vacuum, the value of Λ may change and a supercurvature mode may appear even for $M^2 > 2$, depending on the details of the model. The normalizability conditions may be solved for numerically. In the absence of gravity, there is also a supercurvature mode for the fluctuations of the bubble wall itself, which appears to become singular once gravity is included [26].

III. OVERLAP OF SUPERCURVATURE WITH FLAT MODES FOR A MASSLESS FIELD

We now re-express these supercurvature modes $u_{\Lambda=1\,\ell m}$ in terms of the spatially-flat modes $\phi_{k\ell m}$ for a massless scalar field. There are two things to consider, however, before proceeding to the calculation. First, for $M = 0$, the $\ell = 0$ supercurvature mode of equation (19) is constant. Consequently its Klein-Gordon inner product is zero and its norm (proportional to the square root of the inverse of this norm) diverges as $\Gamma^{1/2}(\ell = 0)$. Including this state naively in the Wightman function sum over states will thus diverge as well. It is known that the Wightman function for a massless, minimally-coupled scalar field in de Sitter spacetime is infrared divergent [10,11], and in this particular slicing, the specific state $u_{\Lambda=1,00}$ appears to be the lone source of the divergence.

The r_c-dependent portion of the equations of motion in region C, are exactly like a $(2,1)$-dimensional spacetime with scale factor $a(r_c) = \cosh r_c$, For positive frequency modes,

$$\left[\frac{1}{a^2(r_c)}\frac{\partial}{\partial r_c}\left(a^2(r_c)\frac{\partial}{\partial r_c}\right) + (1 + p^2) + \frac{\ell(\ell+1)}{a^2(r_c)}\right]\{f_{pl}(r_c)Y_{\ell m}(\Omega)\} = 0 \tag{21}$$

and the 'frequency' ω_{r_c} associated with the time-coordinate may then be written

$$\omega_{r_c}^2 = (1 + p^2) + \frac{\ell(\ell+1)}{a^2(r_c)}, \tag{22}$$

the analogue of $\omega^2 = M^2 + k^2/a^2(t)$. This ω_{r_c} vanishes only for $p = i$ and $\ell = 0$, indicating a zero mode corresponding to the symmetry $\phi \to \phi + \text{constant}$. This zero mode should be replaced by a collective coordinate.[3] [11,18,27] Zero modes have also been identified in the context of two field models in [15]. In the following, we address only the finite modes ($\ell > 0$) for the massless, minimally-coupled case.

The only Cauchy surface for the entire de Sitter spacetime in region F is the limiting curve $\eta \to 0$, corresponding to $t_r \to \infty$. This is in contrast with region C where any 'time' $r_c = \text{constant}$ surface is a Cauchy surface. However, all of

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[3]Such divergences do not directly affect CMB anisotropy calculations, which correspond to $\ell > 0$.

region R, containing our open observable universe in models of open inflation, is contained within region F. Because our aim is to provide a useful heuristic relation between the unusual supercurvature modes and the more familiar spatially-flat modes, we will thus work in this section at fixed time within region F. Verifying these results, Appendix B contains a parallel calculation for all odd ℓ and $\ell = 2$ along the proper Cauchy surface $r_c = 0$. In Appendix C the overlap for $\ell = 1$ is found on the boundary of F, corresponding to Cauchy surface $\eta = 0$.

The Klein-Gordon inner product in region F is

$$(u,\, v) = -ia^2(\eta) \int_0^\infty dr_f\, r_f^2 \int d\Omega \left[u\left(\partial_\eta \overline{v}\right) - \left(\partial_\eta u\right) \overline{v} \right]_\Sigma . \tag{23}$$

This can be evaluated along any fixed-η surface Σ, and, if the fields fall off sufficiently quickly on the time-like boundaries, will be independent of the specific choice of η, even though such fixed-η surfaces are not Cauchy surfaces for the entire spacetime. The modes $\phi_{k\ell m}(x_f)$ and $\overline{\phi}_{k\ell m}(x_f)$ satisfy the inner product relations of equation (9) along such fixed-η surfaces within region F, and form a complete set of orthonormalized modes within region F; thus they may be used to expand any normalizable function within region F. The massless supercurvature mode $u_{\Lambda=1,\ell'm'}$ is normalizable on fixed η surfaces with $-1 \le \eta \le 0$, as shown in Appendix A. Its norm being independent of η suggests that its falloff is fast enough to make the inner products independent of η as well. Thus we expect we can express the massless supercurvature mode $u_{\Lambda=1,\ell'm'}(x_r(x_f))$ in terms of the flat basis functions as

$$u_{\Lambda=1,\ell'm'}(x_r(x_f)) = \int_0^\infty dk \sum_{\ell,m} \left[\alpha_{k\ell m}\, \phi_{k\ell m}(x_f) + \beta_{k\ell m}\, \overline{\phi}_{k\ell m}(x_f) \right], \tag{24}$$

with $\alpha_{k\ell m}$ and $\beta_{k\ell m}$ constant complex coefficients,

$$\alpha_{k\ell m} = \left(u_{\Lambda=1,\ell m},\, \phi_{k\ell m} \right) \;,\quad \beta_{k\ell m} = -\left(u_{\Lambda=1,\ell m},\, \overline{\phi}_{k\ell m} \right), \tag{25}$$

even for a fixed η (non-Cauchy) surface.

For $M = 0$, the spatially-flat basis modes (equation (11)) reduce to

$$\phi_{k\ell m}(x_f) = \frac{i}{\sqrt{\pi k}}(1 + ik\eta)e^{-ik\eta} j_\ell(kr_f) Y_{\ell m}(\Omega)$$
$$\equiv \frac{i}{\sqrt{\pi k}} F_{k\ell}(\eta, r_f) Y_{\ell m}(\Omega), \tag{26}$$

and the normalized supercurvature modes for the massless case are

$$u_{\Lambda=1,\ell m}(x_r) = \frac{1}{2}\sqrt{\Gamma(\ell)\Gamma(\ell+2)}\, \frac{P_{-3/2}^{-\ell-1/2}(\cosh r_r)}{\sqrt{\sinh r_r}}\, Y_{\ell m}(\Omega)$$
$$\equiv \frac{1}{2}\sqrt{\Gamma(\ell)\Gamma(\ell+2)}\, S_\ell(r_r)\, Y_{\ell m}(\Omega) \tag{27}$$

within region R. Using the embedding coordinates z^μ of the five-dimensional Minkowski space to relate the coordinates x_f and x_r (see equations (2) and (4)) yields

$$\cosh r_r = \frac{g}{\sqrt{g^2-1}} \;, \;\; \sinh r_r = \frac{1}{\sqrt{g^2-1}} \;, \tag{28}$$

where

$$g = g(\eta, r_f) \equiv \frac{1}{2r_f}\left(1 + r_f^2 - \eta^2\right). \tag{29}$$

The coordinate g is convenient because of the identities (see [25], equations 8.2.7 and 8.6.7):

$$P_{-\beta-1/2}^{-\alpha-1/2}\left(\frac{z}{\sqrt{z^2-1}}\right) = \sqrt{\frac{2}{\pi}}\frac{(z^2-1)^{1/4}\, e^{-i\beta\pi}\, Q_\alpha^\beta(z)}{\Gamma(\alpha+\beta+1)},$$

$$Q_\ell^1(z) = \sqrt{z^2-1}\,\frac{dQ_\ell(z)}{dz}, \tag{30}$$

where $Re\,[z] > 0$. Taking $g = z$ and noting that $0 \le r_f \le \infty$ in the inner product means that we want fixed η surfaces with $-1 \le \eta \le 0$. When $z^2 = g^2 < 1$, the argument of $P_{-\beta-1/2}^{-\alpha-1/2}$ becomes complex and hence the righthand side should be understood with z having a small imaginary part. Unless $\eta = 0$, fixing η and letting r_f range over its values $0 \le r_f \le \infty$ will include some values of $g^2 < 1$.

With the identities (30) above,

$$S_\ell(r_r) = \frac{P_{-3/2}^{-\ell-1/2}(\cosh r_r)}{\sqrt{\sinh r_r}} = -\sqrt{\frac{2}{\pi}}\frac{1}{\Gamma(\ell+2)}\left(g^2-1\right)\partial_g Q_\ell(g), \tag{31}$$

and the overlap in equation (25) is then

$$\alpha_{k\ell m} = -\mathcal{C}_{k\ell}(-\eta)^{-2}e^{ik\eta}\int_0^\infty dr_f\, r_f^2\, j_\ell(kr_f)\left[k^2\eta\, S_\ell(r_r(x_f)) - (1-ik\eta)\partial_\eta S_\ell(r_r(x_f))\right]_\Sigma,$$

$$\mathcal{C}_{k\ell} \equiv \frac{1}{2}\left[\frac{\Gamma(\ell)\Gamma(\ell+2)}{\pi k}\right]^{1/2}. \tag{32}$$

Note that the constant coefficients $\mathcal{C}_{k\ell}$ are purely real. Similarly,

$$\beta_{k\ell m} = \mathcal{C}_{k\ell}(-\eta)^{-2}e^{-ik\eta}(-1)^m\delta_{m,-m'}\left[k^2\eta - (1+ik\eta)\partial_\eta\right]\int_0^\infty dr_f\left[r_f^2\, j_\ell(kr_f)S_\ell(r_r)\right]_\Sigma. \tag{33}$$

As both $\phi(x_f), u(x_r)$ correspond to positive frequency for the Bunch-Davies vacuum, $\beta_{k\ell m} = 0$ for all k, ℓ, and m, giving

$$\partial_\eta I_\ell(k)_{|\Sigma} = \frac{k^2\eta}{(1+ik\eta)}\, I_\ell(k)_{|\Sigma},$$

$$I_\ell(k)_{|\Sigma} \equiv \int_0^\infty dr_f\left[r_f^2\, j_\ell(kr_f)S_\ell(r_r)\right]_\Sigma, \tag{34}$$

or

$$\alpha_{k\ell m} = -2i\mathcal{C}_{k\ell}k^3\frac{e^{ik\eta}}{(1+ik\eta)}I_\ell(k)_{|\Sigma}. \tag{35}$$

Equation (34) may be used to demonstrate explicitly that $\partial_\eta \alpha_{k\ell m} = 0$ identically, allowing a choice of any convenient value of η to evaluate $I_\ell(k)$. We choose $\eta = -1$ in this section; the case $\eta = 0$ and $\ell = 1$ is in Appendix C.

Along the surface $\eta = -1$, $g_* = r_f/2$ and

$$I_\ell(k)_{|\Sigma} = -8\sqrt{\frac{2}{\pi}} \frac{1}{\Gamma(\ell+2)} \int_0^\infty dg_*\, g_*^2 \left(g_*^2 - 1\right)\, j_\ell(2kg_*)\frac{dQ_\ell(g_*)}{dg_*}, \tag{36}$$

where the $*$ indicates that a particular value of η has been chosen for this evaluation. For several small values of ℓ, repeated integration by parts gives the general form (dropping the subscript $*$)

$$\int dg\, g^2 \left(g^2 - 1\right) j_\ell(2kg)\partial_g Q_\ell(g) = a_1\, \cos(2kg) + a_2\, \sin(2kg)$$
$$+ a_3\, (\text{ci}\,[2k(1+g)] - \text{ci}\,[2k(1-g)])$$
$$+ a_4\, (\text{Si}\,[2k(1+g)] - \text{Si}\,[2k(1-g)])$$
$$+ a_5\, \text{Si}\,[2kg], \tag{37}$$

where $\text{ci}\,(z) \equiv -\int_z^\infty dt\, \frac{\cos t}{t}$, $\text{Si}\,(z) \equiv \int_0^z dt\, \frac{\sin t}{t}$, and generally $a_i = a_i(g,k)$. For $\ell = 1$, the nonzero coefficients are

$$a_1 = \frac{g}{2k^3} + \frac{1}{8k^5}\ln\left(\frac{g+1}{g-1}\right)\left[1 + k^2 - 2k^2 g^2\right],$$
$$a_2 = \frac{(k^2 g^2 - 2)}{4k^4} + \frac{1}{8k^4}\ln\left(\frac{g+1}{g-1}\right)\left[2g + k^2 g\left(1 - g^2\right)\right],$$
$$a_3 = \frac{1}{8k^5}\left[(k^2 - 1)\,\cos(2k) - 2k\,\sin(2k)\right],$$
$$a_4 = \frac{1}{8k^5}\left[2k\,\cos(2k) + (k^2 - 1)\,\sin(2k)\right]. \tag{38}$$

Using [25,28], as $g \to \infty$, $a_1 \to 0$ and $a_2 \to (6k^2)^{-1}$ and thus

$$\int_0^\infty dg\, g^2 \left(g^2 - 1\right) j_1(2kg)\partial_g Q_1(g) = \frac{1}{6k^2}\sin(2kg)_{g\to\infty} + \frac{\pi(1 - ik)e^{ik}}{4k^5}\left[k\,\cos(k) - \sin(k)\right]. \tag{39}$$

Based on comparison with the explicit calculation of this definite integral along different surfaces (see Appendix B), we drop the first term, as its limiting value oscillates at $g \to \infty$. Then the coefficient of expansion $\alpha_{k,\ell=1,m}$ becomes

$$\alpha_{k,\ell=1,m} = -2i\, k^{-1/2}\, j_1(k). \tag{40}$$

Repeating the same analysis for $\ell = 2, 3$, for which a_1 and a_2 both vanish identically as $g \to \infty$, yields

$$\alpha_{k,\ell=2,m} = -2i\sqrt{3}\, k^{-1/2}\, j_2(k),$$
$$\alpha_{k,\ell=3,m} = -2i\sqrt{6}\, k^{-1/2}\, j_3(k). \tag{41}$$

These first three expansion coefficients are plotted in Figure 3.
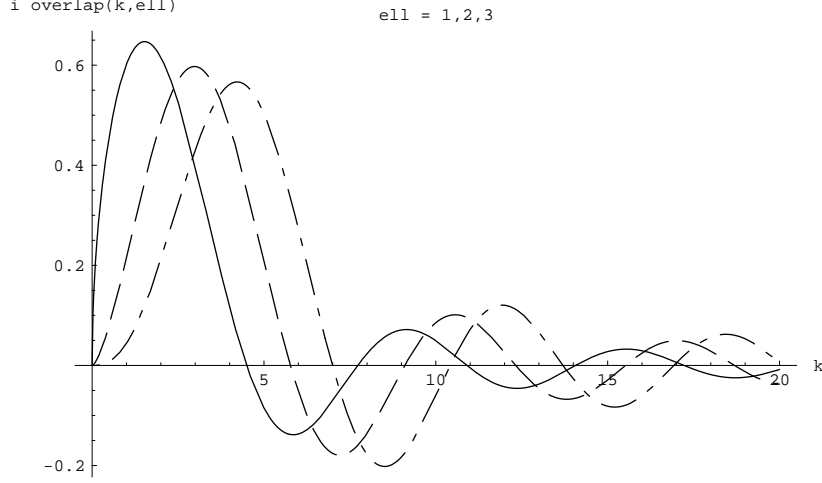
FIG. 3. The first three expansion coefficients, $i\alpha_{k\ell m}$ for $\ell = 1, 2, 3$, plotted against wavenumber k of the modes in the spatially-flat slicing, x_f.

These coefficients are finite in both the $k \to 0$ and $k \to \infty$ limits,

$$\lim_{k\to 0} k^{-1/2} j_\ell(k) \sim \text{constant } k^{\ell-1/2} \to 0 \quad (\text{for } \ell > 0) \tag{42}$$

$$\lim_{k\to\infty} k^{-1/2} j_\ell(k) \sim \text{constant } k^{-3/2} \sin\left(k - \frac{\pi\ell}{2}\right) \to 0 \tag{43}$$

by the asymptotics of spherical Bessel functions (*e.g.* [25], equations 10.1.4, and 9.2.5).

Equations (40,41) suggest that the general form for the overlap of the supercurvature modes with the flat basis functions is proportional to $j_\ell(k)k^{-1/2}$. This can be tested by seeing if these postulated $\alpha_{k\ell m}$ reconstruct the supercurvature mode, *i.e.*

$$u_{\Lambda=1,\ell m}(x_r) = \int_0^\infty dk\, \alpha_{k\ell m}\, \phi_{k\ell m}\ . \tag{44}$$

The most convenient choice of η for this integral is the surface $\eta = 0$, since in this case the k dependence in $\phi_{\ell m}$ is proportional to $j_\ell(kr_f)k^{-1/2}$. Writing $\alpha_{k\ell m} = \mathcal{D}_\ell\, k^{-1/2}\, j_\ell(k)$ and substituting into equation (44), we have

$$\frac{1}{2}\sqrt{\Gamma(\ell)\Gamma(\ell+2)}\, S_\ell(r_r(\eta = 0)) =^? \frac{i}{\sqrt{\pi}} \mathcal{D}_\ell \int_0^\infty dk\, \frac{j_\ell(kr_f)j_\ell(k)}{k}. \tag{45}$$

For the left hand side of this equation, using equation (29) and setting $\eta = 0$,

$$S_\ell(r_r(\eta = 0)) = \sqrt{\frac{1-r_f^2}{2r_f}}\, P_{-3/2}^{-\ell-1/2}\left(\frac{1+r_f^2}{1-r_f^2}\right). \tag{46}$$

Region R corresponds to $z^4 \geq 1$, which requires $r_f^2 \leq 1$ as $\eta \to 0$.

12

The right hand side of equation (45) can be integrated to give ([25], equation 11.4.34):

$$\int_0^\infty dk \, \frac{j_\ell(kr_f)j_\ell(k)}{k} = \frac{\sqrt{\pi}}{4} \frac{r_f^\ell \, \Gamma(\ell)}{\Gamma(\ell+3/2)} \, F\left(\ell, -1/2; \ell+3/2; r_f^2\right),\tag{47}$$

where $F(a,b;c;z)$ is the hypergeometric function. By using $F(a,b;c;z) = F(b,a;c;z)$, the representation of $P_\nu^\mu(z)$ in terms of hypergeometric functions ([28], equation 8.772.3), and $P_\nu^\mu(z) = P_{-\nu-1}^\mu(z)$, the righthand side of equation (45) becomes

$$\frac{\sqrt{\pi}}{4} \frac{r_f^\ell \, \Gamma(\ell)}{\Gamma(\ell+3/2)}\Gamma(\ell+3/2) \, r_f^{-\ell-1/2} \sqrt{1-r_f^2} \, P_{-3/2}^{-\ell-1/2}\left(\frac{1+r_f^2}{1-r_f^2}\right) =$$
$$\frac{\sqrt{\pi}}{4}\Gamma(\ell)\sqrt{\frac{1-r_f^2}{r_f}} \, P_{-3/2}^{-\ell-1/2}\left(\frac{1+r_f^2}{1-r_f^2}\right).\tag{48}$$

Thus the r_f dependence on both sides of equation (45) matches exactly, and the constant $\mathcal{D}_\ell$ may be read off:

$$\mathcal{D}_\ell = -i\sqrt{2\ell(\ell+1)}.\tag{49}$$

This coefficient reproduces the specific $\alpha_{k\ell m}$ calculated earlier for $\ell = 1$, 2, 3 along the surface $\eta = -1$. Resumming the equation for $r_f > 1$ would correspond to region L in de Sitter space.

Thus we conclude that the constant coefficients $\alpha_{k\ell m}$ which relate the normalized supercurvature modes $u_{\Lambda\ell m}$ and the spatially-flat basis modes $\phi_{k\ell m}$ are:

$$\alpha_{k\ell m} = -i\sqrt{2\ell(\ell+1)} \, k^{-1/2} \, j_\ell(k).\tag{50}$$

This is the main result of this paper.

Taking the limit $r_f \to 1$ in equation (47), and using the identity ([28], equation 9.122.1):

$$F(\alpha, \beta, \gamma; 1) = \frac{\Gamma(\gamma)\Gamma(\gamma-\alpha-\beta)}{\Gamma(\gamma-\alpha)\Gamma(\gamma-\beta)},\tag{51}$$

it is easy to verify in addition that

$$\int_0^\infty dk \, |\alpha_{k\ell m}|^2 = 2\ell(\ell+1) \int_0^\infty dk \, \frac{j_\ell(k)j_\ell(k)}{k} = 1.\tag{52}$$

IV. CONCLUSION

In conclusion, we have given the explicit form for the overlap between the flat basis functions (26) and the massless supercurvature modes. As a result, the supercurvature modes within that patch of de Sitter space which would contain our open observable universe can be written

$$u_{\Lambda=1\,\ell m}(x_r(x_f)) = -i\sqrt{2\ell(\ell+1)} \int_0^\infty dk \, k^{-1/2} \, j_\ell(k) \, \phi_{k\ell m}(x_f). \tag{53}$$

The long-wavelength supercurvature modes are distributed over the spatially-flat basis modes, oscillating over flat-space comoving wavenumber k with decreasing amplitude. More quantitatively, the spherical bessel functions $j_\ell(k)$ have their first and largest maximum ([25] 10.1.59) near $k \sim (\ell + \frac{1}{2})[1 + O(\ell^{-2/3})]$ with the approximation improving as ℓ increases, but the damping envelope going as $k^{-1/2}$ lowers this peak for higher ℓ. It may be possible to use the description [15] of $M^2 \neq 0$ supercurvature modes as small perturbations of the massless supercurvature modes to extend the above to small M^2.

This expression for the supercurvature mode on fixed η surfaces, extending into region R, may be useful for understanding the effects of supercurvature modes during reheating. Unlike the event of bubble nucleation, reheating occurs in the future of region C and hence descriptions using fixed time r_c surfaces are not appropriate. Rather, it is important to understand the dynamics of these modes within region R, corresponding to our observable, open universe. Having an expression for the normalizable supercurvature modes on slicings extending into region R is a step in separating long wavelength properties of these modes from issues related to their non-normalizability at fixed time t_r in region R.

We showed by comparing Cauchy and non-Cauchy surface calculations that in some cases non-Cauchy surface calculations of norms (in the appendix) and overlaps (in the text) agree for supercurvature modes, up to an identifiable boundary term. These non-Cauchy surfaces (fixed time in the flat coordinates) extend into the open universe and thus could be used (with caution) to calculate other properties. The complementary calculations along different surfaces were required to verify that the non-Cauchy surface representation was indeed correct.

In addition, we identify one specific supercurvature mode as responsible for the well-known infrared divergence for massless scalar fields in de Sitter space. Not only does this mode have divergent norm; it is demonstrated here to be a dynamical zero-mode. This identification is a necessary first step toward its eventual replacement with an appropriate collective coordinate, similar to what has been done in closed coordinates [11]. Something similar has been done in [15] in the context of two field models and quasi-open inflation, here it is found more generally as a property of the massless supercurvature modes.

<h2 style="text-align:center">V. APPENDICES</h2>

<h3 style="text-align:center">A. Normalization of supercurvature mode at fixed time $-1 \leq \eta \leq 0$</h3>

In region F the supercurvature mode can be written as (using equation 28)

$$S_\ell(r_r(g)) = \frac{P_{-3/2}^{-\ell-1/2}(\cosh r_r)}{\sqrt{\sinh r_r}} = (g^2 - 1)^{1/4} \, P_{-3/2}^{-\ell-1/2}\left(\frac{g}{\sqrt{g^2 - 1}}\right) \tag{54}$$

which can be used to extend out of region R, to where $g \leq 1$. We will consider only $-1 \leq \eta \leq 0$ for convenience.

The inner product for fixed time η is

$$(S_\ell, \, S_\ell) = -ia^2(\eta) \int_0^\infty dr_f \, r_f^2 \int d\Omega \left[S_\ell \left(\partial_\eta \overline{S}_\ell \right) - (\partial_\eta S_\ell) \, \overline{S}_\ell \right]_\Sigma. \tag{55}$$

The integral over Ω gives a delta function and will be suppressed.

For $g \geq 1$, $S_\ell = \overline{S}_\ell$ because both the associated Legendre function and its argument are real, and so the integrand disappears. For fixed η, $g^2 = 1$ corresponds to

$$(1 - r_f)^2 = \eta^2 \Rightarrow r_f = 1 \pm \eta . \tag{56}$$

With $-1 \leq \eta \leq 0$, the integral is

$$(S_\ell, \, S_\ell) = i\frac{1}{\eta} \int_{1+\eta}^{1-\eta} dr_f \, r_f \left[S_\ell \left(\partial_g \overline{S}_\ell \right) - (\partial_g S_\ell) \, \overline{S}_\ell \right]_\Sigma. \tag{57}$$

where we have substituted as well $\partial_\eta f(g) = -(\eta/r_f)\partial_g f(g)$ and $a^2(\eta) = \eta^{-2}$. In the region of integration, we also have $\overline{S_\ell(g)} = S_\ell(-g)$. Inside the integral, the terms where the derivatives act on $(g^2 - 1)^{1/4}$ and its complex conjugate cancel out. Defining $y = g/\sqrt{g^2 - 1}$,

$$\begin{aligned}
S_\ell \left(\partial_\eta \overline{S}_\ell \right) - (\partial_\eta S_\ell) \, \overline{S}_\ell &= |g^2 - 1|^{1/2} \frac{dy}{dg} \left[P_{-3/2}^{-\ell-1/2}(y) \left(\partial_y P_{-3/2}^{-\ell-1/2}(-y) \right) \right. \\
&\quad \left. - \left(\partial_y P_{-3/2}^{-\ell-1/2}(y) \right) P_{-3/2}^{-\ell-1/2}(-y) \right]
\end{aligned} \tag{58}$$

So we are left with the wronskian of $P_{-3/2}^{-\ell-1/2}(y)$ and $P_{-3/2}^{-\ell-1/2}(-y)$ times $dy(g)/dg$. We can now use ([28], equations 8.736.2, 8.334.3, 8.335.1, and [25], equation 8.1.8)

$$\begin{aligned}
P_\nu^\mu(y) \frac{d}{dy} P_\nu^\mu(-y) - \frac{d}{dy} P_\nu^\mu(y) P_\nu^\mu(-y) &= -\frac{2}{\pi} \sin[(\mu+\nu)\pi] e^{-\mu\pi i} [P_\nu^\mu(y) \frac{d}{dy} Q_\nu^\mu(y) - \frac{d}{dy} P_\nu^\mu(y) Q_\nu^\mu(y)] \\
&= -\frac{2}{\pi} \sin[(\nu+\mu)\pi] \frac{2^{2\mu} \Gamma(\frac{\mu+\nu+2}{2}) \Gamma(\frac{\mu+\nu+1}{2})}{(1-y^2)\Gamma(\frac{-\mu+\nu+2}{2})\Gamma(\frac{-\mu+\nu+1}{2})} \\
&= -\frac{1}{2^{2\ell}\pi} \sin[-(\ell+2)\pi] \frac{\Gamma(\frac{-\ell}{2})\Gamma(\frac{-\ell-1}{2})}{(1-y^2)\Gamma(\frac{\ell+1}{2})\Gamma(\frac{\ell}{2})} \\
&= -\frac{2}{(1-y^2)\pi} \sin[-(\ell+2)\pi] \frac{\Gamma(-\ell-1)}{\Gamma(\ell)} \\
&= \frac{2}{(1-y^2)} \frac{1}{\Gamma(\ell)\Gamma(\ell+2)} .
\end{aligned} \tag{59}$$

Including

$$\frac{d}{dg} y(g) = -\frac{1}{(g^2-1)^{3/2}} , \tag{60}$$

using $|g^2 - 1|^{1/2}/(g^2 - 1)^{1/2} = i$, and substituting the above, the inner product becomes

15

$$\frac{i}{\eta} \int_{1+\eta}^{1-\eta} dr_f \, r_f \left[S_\ell \left(\partial_g \overline{S}_\ell \right) - \left(\partial_g S_\ell \right) \overline{S}_\ell \right]_\Sigma = -\frac{2}{\Gamma(\ell)\Gamma(\ell+2)} \frac{1}{\eta} \int_{1+\eta}^{1-\eta} dr_f \, r_f$$

$$= -\frac{2}{\Gamma(\ell)\Gamma(\ell+2)} \frac{1}{\eta} \left[\frac{(1-\eta)^2}{2} - \frac{(1+\eta)^2}{2} \right]$$

$$= \frac{4}{\Gamma(\ell)\Gamma(\ell+2)} \tag{61}$$

which is independent of η as promised. This also shows that the supercurvature modes are properly normalized for fixed time surfaces $-1 \leq \eta \leq 0$ in region F. This suggests that at spatial infinity in the flat coordinates the supercurvature modes have sufficiently fast falloff to correspond to their inner product on a Cauchy surface. (This is not true for fixed time surfaces in region R for example, as the supercurvature modes diverge at spatial infinity.)

B. Overlap along $r_c = 0$, for ℓ odd and $\ell = 2$

In region C the inner product (equation (10)) is

$$(u, v) = -i \cosh^2 r_c \int_{-\pi/2}^{\pi/2} dt_c \cos t_c \int d\Omega \left(\frac{\partial u}{\partial r_c} \overline{v} - u \frac{\partial \overline{v}}{\partial r_c} \right) \tag{62}$$

and will be taken on the Cauchy surface $r_c = 0$. From their definitions, equations (2) and (4), the spatially-flat coordinates and the region C coordinates are related via

$$r_f = \frac{\cos t_c \cosh r_c}{\sin t_c + \cos t_c \sinh r_c}$$

$$\eta = -\frac{1}{\sin t_c + \cos t_c \sinh r_c} , \tag{63}$$

with $t_c > 0$. For $t_c < 0$ we need the analytic continuation of the basis function

$$\phi_{k\ell m}(x_f(r_c, t_c)) = \frac{i}{\sqrt{\pi k}} \left(1 + ik\eta(r_c, t_c) \right) e^{-ik\eta(r_c, t_c)} j_\ell(kr_f(r_c, t_c)) Y_{\ell m}(\Omega). \tag{64}$$

As this basis function has no branch cuts as a function of $r_f(r_c, t_c), \eta(r_c, t_c)$, the continuation to $t_c < 0$ is straightforward and the same for both positive and negative frequency mode functions.

Using $\phi_{k\ell m}(x)$ to denote both the function in region F and its analytic continuation into region $t_c < 0$, the inner product $\alpha_{k\ell m}$ between $u_{\Lambda=1\,\ell m}$ and ϕ is

$$(u_{\Lambda=1\,\ell m}, \phi_{k\ell' m'}) = -i \int_{-\pi/2}^{\pi/2} dt_c \cos t_c \int d\Omega$$

$$\times \left[u_{\ell m}(r_c, \Omega) \left(\partial_{r_c} \overline{\phi}_{k\ell' m'}(\eta, r_f, \Omega) \right) - \left(\partial_{r_c} u_{\ell m}(r_c, \Omega) \right) \overline{\phi}_{k\ell' m'} \right] |_{r_c=0} . \tag{65}$$

For ease of calculation, we take

$$\phi_{k\ell m}(x) = \frac{i}{\sqrt{\pi k}} F_{k\ell}(x) Y_{\ell m}(\Omega)$$

$$u_{\Lambda=1\,\ell m}(x_c) = \frac{1}{2} \sqrt{\Gamma(\ell)\Gamma(\ell+2)} \, S_\ell(r_c) Y_{\ell m}(\Omega) \tag{66}$$

16

The integral over $d\Omega$ is immediate, giving $\delta_{mm'}\delta_{\ell\ell'}$, and we suppress these delta functions in the following. Pulling out normalization factors, the inner product becomes

$$\alpha_{k\ell m} = -A(\ell, k) \int_{-\pi/2}^{\pi/2} dt_c \cos t_c \left[S_\ell(r_c) \left(\partial_{r_c} \overline{F}_{k\ell}(\eta, r_f) \right) - \left(\partial_{r_c} S_\ell(r_c) \right) \overline{F}_{k\ell}(\eta, r_f) \right] |_{r_c=0} , \tag{67}$$

where $A(\ell, k) \equiv \frac{1}{2} \sqrt{\ell(\ell+1)} \Gamma(\ell)/\sqrt{\pi k}$.

For $M = 0$, $S_\ell(r_c)$ is independent of space t_c and can be pulled out of the integral to give

$$(u_{\Lambda=1\,\ell m}, \phi_{k\ell m}) = -A(\ell, k)\{S_\ell(r_c)\partial_{r_c} - \partial_{r_c}S_\ell(r_c)\} \int_{-\pi/2}^{\pi/2} dt_c \cos t_c \overline{F}_{k\ell}(\eta, r_f)|_{r_c=0} . \tag{68}$$

Taking the limit $r_c \to 0$ (and remembering that $P_{-3/2}^{-\ell-1/2}$ has imaginary argument) one has ([25], equation 8.1.4)

$$\begin{aligned}
S_\ell(0) &= \frac{P_{-3/2}^{-\ell-1/2}(i\sinh r_c)}{\sqrt{i\cosh r_c}}\Big|_{r_c=0} = e^{-i\pi/4} e^{\pi i(\ell/2+1/4)} \frac{2^{-\ell-1/2}\sqrt{\pi}}{\Gamma(\frac{\ell+1}{2})\Gamma(\frac{\ell+3}{2})} \\
&\equiv e^{\pi i\ell/2} B(\ell)
\end{aligned} \tag{69}$$

and

$$\begin{aligned}
\partial_{r_c} S_\ell(r_c)|_{r_c=0} &= \partial_{r_c} \left[\frac{P_{-3/2}^{-\ell-1/2}(i\sinh r_c)}{\sqrt{i\cosh r_c}} \right]_{r_c=0} \\
&= \frac{\ell P_{-1/2}^{-\ell-1/2}(i\sinh r_c)}{(i\cosh r_c)^{3/2}}\Big|_{r_c=0} = \frac{e^{-3i\pi/4} e^{\pi i(\ell/2+1/4)} \ell \, 2^{-\ell-1/2}\sqrt{\pi}}{(\Gamma(\frac{\ell+2}{2}))^2} \\
&\equiv e^{\pi i(\ell/2-1/2)} C(\ell) .
\end{aligned} \tag{70}$$

The inner product now becomes

$$\alpha_{k\ell m} = -i^\ell A(\ell, k)\{B(\ell)\partial_{r_c} + iC(\ell)\} \int_{-\pi/2}^{\pi/2} dt_c \cos t_c \overline{F}_{k\ell}(\eta, r_f)|_{r_c=0} , \tag{71}$$

where $A(\ell), B(\ell), C(\ell)$ are all real.

Again, both $u_{\Lambda=1\,\ell m}$ and $\phi_{k\ell m}$ are positive-frequency mode functions for the Bunch-Davies vacuum, so that $\beta_{k\ell m}$ (defined in equation (25)) vanishes:

$$\begin{aligned}
0 &= (u_{\Lambda=1\,\ell m}, \overline{\phi}_{k\ell'm'}) \\
&= -i^\ell A(\ell, k)(-1)^{m+1}\delta_{m',-m}\{B(\ell)\partial_{r_c} + iC(\ell)\} \int_{-\pi/2}^{\pi/2} dt_c \cos t_c F_{k\ell}(\eta, r_f)|_{r_c=0} ,
\end{aligned} \tag{72}$$

The complex conjugate of this equation implies

$$B(\ell)\partial_{r_c} \int_{-\pi/2}^{\pi/2} dt_c \cos t_c \overline{F}_{k\ell}(\eta, r_f)|_{r_c=0} = iC(\ell) \int_{-\pi/2}^{\pi/2} dt_c \cos t_c \overline{F}_{k\ell}(\eta, r_f)|_{r_c=0} . \tag{73}$$

Defining

17

$$\overline{\mathcal{I}}_\ell(k) \equiv \int_0^{\pi/2} dt_c \cos t_c \overline{F}_{k\ell}(\eta, r_f)|_{r_c=0} \tag{74}$$

and using that $j_\ell(kr) = (-1)^\ell j_\ell(-kr)$ is real,

$$\begin{aligned}
\overline{F}_{k\ell}(x_f(-t_c))|_{r_c=0} &= \left(1 - i\frac{k}{\sin(-t_c)}\right) e^{i\frac{k}{\sin(-t_c)}} j_\ell(k\cot(-t_c)) \\
&= \left(1 + i\frac{k}{\sin(t_c)}\right) e^{-i\frac{k}{\sin(t_c)}} (-1)^\ell j_\ell(k\cot(t_c)) \\
&= (-1)^\ell F_{k\ell}(x_f(t_c))|_{r_c=0} .
\end{aligned} \tag{75}$$

Thus we can write

$$\partial_{r_c} \int_{-\pi/2}^{\pi/2} dt_c \cos t_c \overline{F}_{k\ell}(\eta, r_f)|_{r_c=0} = i\frac{C(\ell)}{B(\ell)}(\overline{\mathcal{I}}_\ell(k) + (-1)^\ell \mathcal{I}_\ell(k)) . \tag{76}$$

Substituting in, the full inner product is thus

$$\begin{aligned}
(u_{\Lambda=1\,\ell m}, \phi_{k\ell m}) &= -2i^{\ell+1} C(\ell) A(\ell, k)(\overline{\mathcal{I}}_\ell(k) + (-1)^\ell \mathcal{I}_\ell(k)) \\
&= -i^{\ell+1} \frac{\ell\, 2^{-\ell-1/2}\sqrt{\pi}}{(\Gamma(\frac{\ell+2}{2}))^2} \sqrt{\ell(\ell+1)} \frac{\Gamma(\ell)}{\sqrt{\pi k}} (\overline{\mathcal{I}}_\ell(k) + (-1)^\ell \mathcal{I}_\ell(k)) \\
&= -\frac{i^{\ell+1}}{\sqrt{k}} \frac{2^{-\ell-1/2}\,\ell\,\sqrt{\ell(\ell+1)}\Gamma(\ell)}{(\Gamma(\frac{\ell+2}{2}))^2} (\overline{\mathcal{I}}_\ell(k) + (-1)^\ell \mathcal{I}_\ell(k)).
\end{aligned} \tag{77}$$

The calculation of the inner product thus requires the integral

$$\mathcal{I}_\ell(k) = \int_0^{\pi/2} dt_c \cos t_c (1 + ik\eta) e^{-ik\eta} j_\ell(kr_f)|_{r_c=0} . \tag{78}$$

Changing coordinates and expressing η, t_c in terms of r_f (there is only one free coordinate as r_c has been fixed to zero), using

$$\eta = -\sqrt{r_f^2 + 1} , \quad \tan t_c = \frac{1}{r_f}, \tag{79}$$

gives

$$\mathcal{I}_\ell(k) = \int_0^\infty dr_f \frac{r_f}{(r_f^2+1)^{3/2}} \left(1 - ik\sqrt{r_f^2+1}\right) e^{ik\sqrt{r_f^2+1}} j_\ell(kr_f) . \tag{80}$$

To proceed, note

$$\frac{r_f}{(r_f^2+1)^{3/2}} \left(1 - ik\sqrt{r_f^2+1}\right) e^{ik\sqrt{r_f^2+1}} = -\partial_{r_f}\left(\frac{e^{ik\sqrt{r_f^2+1}}}{\sqrt{r_f^2+1}}\right) . \tag{81}$$

For ℓ odd, we need the imaginary part of $\mathcal{I}_\ell(k)$ and so can use ([25], equation 10.1.45)

18

$$\frac{i \sin k\sqrt{r_f^2+1}}{k\sqrt{r_f^2+1}} = i\sum_{n=0}^{\infty}(2n+1)j_n(kr_f)j_n(k)P_n(0) \tag{82}$$

Consequently, for ℓ odd the integral of interest is

$$\text{Im } \mathcal{I}_{\ell,odd}(k) = -ik\sum_{n=0}^{\infty}(2n+1)j_n(k)P_n(0)\int_0^{\infty}dr_f\partial_{r_f}(j_n(kr_f))j_\ell(kr_f) \tag{83}$$

Using Mathematica,

$$\int_0^{\infty}dr\partial_r j_n(kr_f)j_\ell(kr_f) = \frac{\ell(\ell+1)-n(n+1)}{(\ell-n-1)(\ell-n+1)(\ell+n)(2+\ell+n)}\cos[\pi\frac{\ell-n}{2}]$$

$$(\ell \text{ odd}) = \frac{\ell(\ell+1)-n(n+1)}{(\ell-n-1)(\ell-n+1)(\ell+n)(2+\ell+n)}\sin\frac{\pi\ell}{2}\sin\frac{\pi n}{2} \tag{84}$$

where it appears that n odd is required as well. However, looking at the sum (equation 83), we see this term is multiplied by $P_n(0)$ which vanishes for n odd. So the only possibility for a nonzero term is if the denominator in this expression vanishes, that is if $\ell = n \pm 1$. Substituting in these values and the definition of the Legendre polynomials we get

$$\text{Im } \mathcal{I}_{\ell,odd}(k) = -ik\frac{-\ell}{2\ell+1}\frac{\pi}{2}P_{\ell-1}(0)(j_{\ell-1}(k)+j_{\ell+1}(k))$$

$$= i\ell\frac{\pi}{2}P_{\ell-1}(0)j_\ell(k) \tag{85}$$

Including the prefactors (equation (78)) and after some algebra with Γ functions one gets that the overlap for ℓ odd is

$$\alpha_{k\ell m} = -i\sqrt{2\ell(\ell+1)}k^{-1/2}j_\ell(k) \quad, \ell \text{ odd} \tag{86}$$

agreeing with equation (50).

For ℓ even the calculation is more involved because the identity required in this case is ([25], equation 10.1.46)

$$\frac{\cos k\sqrt{r_f^2+1}}{k\sqrt{r_f^2+1}} = \begin{cases} -\sum_{n=0}^{\infty}(2n+1)y_n(k)j_n(kr_f)P_n(0) \ , & r_f < 1 \\ -\sum_{n=0}^{\infty}(2n+1)y_n(kr_f)j_n(k)P_n(0) \ , & r_f > 1 \ . \end{cases} \tag{87}$$

so that the range of integration in $\mathcal{I}_\ell(k)$ is split from $0 \leq r_f \leq 1$ and $1 \leq r_f \leq \infty$. As the resummation over $\alpha_{k\ell m}\phi_{k\ell m}$ in equation (45) works equally well for ℓ odd and even, it does not seem enlightening to pursue the calculation for even ℓ in all generality here.

We can check a specific case, $\ell = 2$, by integrating by parts and using the definition of $j_2(kr_f)$,

$$j_2(kr_f) = (kr_f)^2\left(-\frac{1}{k^2r_f}\partial_{r_f}\right)^2\frac{\sin kr_f}{kr_f} \ . \tag{88}$$

to get

19

$$\mathcal{I}_2(k) = \int_0^\infty dr_f \frac{r_f \left(1 - ik\sqrt{r_f^2 + 1}\right)}{(r_f^2 + 1)^{3/2}} e^{ik\sqrt{r_f^2+1}} (kr_f)^2 \left(-\frac{1}{k^2 r_f}\partial_{r_f}\right)^2 \frac{\sin kr_f}{kr_f}$$

$$= -\lim_{r_f \to 0} k^{-3} \frac{r_f \left(1 - ik\sqrt{r_f^2 + 1}\right)}{(r_f^2 + 1)^{3/2}} e^{ik\sqrt{r_f^2+1}} \partial_{r_f} \frac{\sin kr_f}{r_f}$$

$$- k^{-3} \frac{1}{r_f^2}\partial_{r_f} \left[\frac{r_f^2 \left(1 - ik\sqrt{r_f^2 + 1}\right)}{(r_f^2 + 1)^{3/2}} e^{ik\sqrt{r_f^2+1}}\right] \sin kr_f\Big|_0^\infty$$

$$+ k^{-3} \int_0^\infty dr_f \frac{\sin kr_f}{r_f}\partial_{r_f} \left(\frac{1}{r_f}\partial_{r_f} \left[\frac{r_f^2 \left(1 - ik\sqrt{r_f^2 + 1}\right)}{(r_f^2 + 1)^{3/2}} e^{ik\sqrt{r_f^2+1}}\right]\right) . \tag{89}$$

The only nonzero boundary term is the second one, at $r_f = 0$, which can be read off, as it is only nonzero when the derivatives act on r_f rather than on $\sqrt{r_f^2 + 1}$. Substituting $r_f \to \mp(x - x^{-1})/2$ and using Mathematica gives

$$\mathcal{I}_2(k) = \frac{6i(e^{ik} - 1)}{k^3} + \frac{6e^{ik}}{k^2} - i\frac{(1 + 2e^{ik})}{k} . \tag{90}$$

Combining the integral with the prefactors (eqn. (78)), and taking the real part gives

$$\alpha_{k,\ell=2,m} = -i2\sqrt{\frac{3}{k}}\frac{1}{k^3} \left[3\sin k - 3k\cos k - k^2\sin k\right] = -2i\sqrt{3}\, k^{-1/2}\, j_2(k), \tag{91}$$

again in agreement with equation (50).

<div align="center">

C. Overlap along $\eta = 0$, for $\ell = 1$

</div>

Here we discuss the integral (equation (34))

$$I_\ell(k)_{|\Sigma} = \int_0^\infty dr_f \left[r_f^2\, j_\ell(kr_f)S_\ell(r_r)\right]_\Sigma \tag{92}$$

evaluated on the surface in region F corresponding to $\eta = 0$. For $\eta = 0$, $g = (1 + r_f^2)/(2r_f)$ and so

$$I_\ell(k)|_\Sigma = \int_0^\infty dr_f r_f^2 j_\ell(kr_f)(g^2 - 1)\partial_g Q_\ell(g) \tag{93}$$

becomes for $\ell = 1$

$$I_1(k)|_{\eta=0} = -\sqrt{\frac{2}{\pi}}\frac{1}{\Gamma(3)} \int_0^\infty dr_f\, r_f^2 \left[\frac{\sin kr_f}{(kr_f)^2} - \frac{\cos kr_f}{kr_f}\right] \left(\frac{(1 - r_f^2)^2}{8r_f^2} \ln\left(\frac{(1 + r_f)^2}{(1 - r_f)^2}\right) - \frac{1 + r_f^2}{2r_f}\right) \tag{94}$$

This can be rewritten as

$$I_1(k)|_{\eta=0} = -\sqrt{\frac{1}{2\pi}} \int_0^\infty dr_f \left[\frac{\sin kr_f}{(kr_f)^2} - \frac{\cos kr_f}{kr_f}\right] \left(\frac{(1 - r_f^2)^2}{4} \ln\left|\frac{1 + r_f}{1 - r_f}\right| - r_f\frac{1 + r_f^2}{2}\right) \tag{95}$$

and integrated using Mathematica by considering

$$\int_0^1 dr_f \left[\frac{\sin kr_f}{(kr_f)^2} - \frac{\cos kr_f}{kr_f} \right] \left(\frac{(1 - r_f{}^2)^2}{4} \ln\left(\frac{1 + r_f}{1 - r_f} \right) - r_f \frac{1 + r_f{}^2}{2} \right) \tag{96}$$

$$+ \int_1^\infty dr_f \left[\frac{\sin kr_f}{(kr_f)^2} - \frac{\cos kr_f}{kr_f} \right] \left(\frac{(1 - r_f{}^2)^2}{4} \ln\left(\frac{1 + r_f}{-1 + r_f} \right) - r_f \frac{1 + r_f{}^2}{2} \right) \tag{97}$$

$$\tag{98}$$

to get

$$\begin{aligned}
I_1(k) &= -\sqrt{\frac{1}{2\pi}} \{ \lim_{r_f \to \infty} \frac{4}{3k^2} \sin kr_f + \frac{2}{k^5} \left[-(\mathrm{ci}(\infty) - \mathrm{ci}(-\infty))(\cos(k) + k\sin k) \right. \\
&\quad \left. + (\mathrm{Si}(\infty) - \mathrm{Si}(-\infty))(-k\cos k + \sin k) \right] + \frac{2i\pi}{k^5}(\cos k + k\sin k) \} \\
&= -\sqrt{\frac{1}{2\pi}} \left(\lim_{r_f \to \infty} \frac{4}{3k^2} \sin kr_f + -\frac{2\pi}{k^5}(\sin k - k\cos k) \right).
\end{aligned} \tag{99}$$

This gives

$$\alpha_{k,\ell=1,m} = i\frac{k^3}{\sqrt{\pi k}} \left(\lim_{r_f \to \infty} \frac{4}{3k^2} \sin kr_f + -\frac{2\pi}{k^5}(\sin k - k\cos k) \right) = -2ik^{-1/2} \, j_1(k), \tag{100}$$

where the oscillating first term has been dropped as it has the wrong asymptotics as $k \to \infty$. (If $\lim_{r_f \to \infty} \sin kr_f$ was finite rather than the giving zero in this limit, the overlap would diverge as $k \to \infty$.) With this, $\alpha_{k\ell m}$ again agrees with the results found above.

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